Level density and level density parameter in medium heavy nuclei including thermal and quantal fluctuation effects

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Abstract

In a realistic application of the SPA + RPA theory for calculation of the nuclear level densities we find that quantal fluctuation corrections (RPA) are important even up to temperature T=2.0~MeV. This leads to a good agreement between calculated numbers and the available experimental data for ^{104}Pd and ^{114}Sn , particularly the excitation energy (E^*) dependence. Furthermore, we also argue that $a=S^2/4E^*$ is the only correct definition of the level density parameter in the present context which is also consistent with the Bethe like level density formula.

In the last a few years there have been considerable efforts to develop microscopic methods for the calculation of accurate values of level densities as a function of excitation energies[1]-[6]. One of these methods which is of present interest is based on the auxiliary field path integral representation of the partition function for a given nuclear Hamiltonian. The path integral representation can be obtained in two ways: (a) the so called as shell model Monte Carlo (SMMC) method[4, 5] and (b) the SPA+RPA approach [6] which includes the thermal fluctuations through static path approximation (SPA) and the quantal fluctuations about static paths are included using random phase approximation (RPA). It is now well established that SMMC approach can be applied even at very low temperatures. On the otherhand, SPA+RPA approach is computationally faster than SMMC approach and can be used for moderately low to high temperatures, typically, for $T \geq 0.2$ MeV. However, in most of these studies so far the main emphasis has been to demonstrate, through simple model studies, the relative defferences between the SPA and SPA+RPA results for the temperature dependence of the energy and the level density.

Recently[7], the level densities as well as the level density parameters have been extracted for the medium mass nuclei ^{104}Pd through the measurement of proton yields in reaction $^{93}Nb(^{12}C,p)^{104}Pd$ and that of ^{114}Sn through $^{103}Rh(^{12}C,p)^{114}Sn$ reaction. These data are available for the excitation energy (E^*) ranging from 5–25 MeV or equivalently $T \simeq 0.5-1.5~MeV$ which is well suited to test the feasibility of the SPA+RPA approach. In this letter we calculate the level density and the level density parameter as a function of E^* for ^{104}Pd and ^{114}Sn using SPA+RPA approach with a quadrupole-quadrupole interaction model Hamiltonian

$$H = H_0 - \frac{1}{2}\chi \sum_{\mu=-2}^{2} (Q_{\mu})^2. \tag{1}$$

In the above, H_0 represents the spherical part, $Q_0 = Q_0'$, $Q_{+\mu} = \frac{1}{\sqrt{2}}(Q_{\mu}' + Q_{\mu}'^{\dagger})$ and $Q_{-\mu} = \frac{i}{\sqrt{2}}(Q_{\mu}' - Q_{\mu}'^{\dagger})$ with $\mu = 1$ and 2 and Q's stand for the usual quadrupole moment operators. Value of the quadrupole interaction strength $\chi = 120A^{-5/3}f_c$

MeV (A denotes the mass number) is taken from Ref. [8] where $f_c = 1 - 2$ is a core polarization factor.

The grand canonical partition function in SPA+RPA takes the following form [9]

$$\mathcal{Z}_{RPA} = 4\pi^2 \left(\frac{\alpha}{2\pi T}\right)^{5/2} \int \beta^4 d\beta \int |\sin 3\gamma| d\gamma e^{-\frac{\alpha \beta^2}{2T}} \times Tr\left[e^{-H'/T}\right] \mathcal{C}_{RPA}. \tag{2}$$

where, $\alpha = (\hbar\omega_0)^2/\chi$ with $\hbar\omega_0 = 41A^{-1/3}~MeV$. The quantities H' and \mathcal{C}_{RPA} are the single-particle Hamiltonian and the RPA correction factor, respectively, given by

$$H' = H_0 - \hbar\omega_0\beta \left(Q_0 \cos\gamma + Q_{+2} \sin\gamma \right) \tag{3}$$

and

$$C_{RPA} = \left(\prod_{m \neq 0}^{N_m} Det \mid C^m \mid\right)^{-1} \tag{4}$$

with

$$C_{\mu\nu}^{m} = \delta_{\mu\nu} + \chi \sum_{ij} \frac{\langle i \mid Q_{\mu} \mid j \rangle \langle j \mid Q_{\nu} \mid i \rangle}{\Delta_{ij}^{2} + (2\pi mT)^{2}} f_{ij} \Delta_{ij}$$
 (5)

where, $f_{ij} = f_i - f_j$ and $\Delta_{ij} = \epsilon_i - \epsilon_j$ with f_i being the Fermi distribution function and ϵ_i is the eigenvalue of H'. In the above, $|i\rangle$ represents an eigenstate of H'. The grand canonical trace in eq. (2) can simply be performed using

$$Tre^{-\beta'H'} = \left(\prod_{i} \left[1 + e^{-\beta'\epsilon_i + \alpha_p}\right]\right) \left(\prod_{j} \left[1 + e^{-\beta'\epsilon_j + \alpha_n}\right]\right)$$
(6)

where, $\beta' = 1/T$ and $\alpha_p(\alpha_n)$ is the Lagrange multiplier required to adjust the proton(neutron) numbers.

The SPA representation of the partition function can be obtained by putting $C_{RPA} = 1$. It is, therefore, clear from eqs. (4,5) that for higher temperatures $C_{RPA} \longrightarrow 1$ or in other words $Z_{RPA} \longrightarrow Z_{SPA}$.

Once the partition function is known, the level density or more precisely the state density W(E) can be calculated using saddle point approximation which

gives

$$W(E) = \frac{e^S}{(2\pi)^{3/2} \mathcal{D}^{1/2}} \tag{7}$$

where,

$$S = \ln Z + \beta' E - \alpha_p N_p - \alpha_n N_n \tag{8}$$

is the entropy with \mathcal{Z} being the grand canonical partition function in the SPA or SPA+RPA approach. The quantities $\alpha_{p,n}$ and β' (or T^{-1}) are so chosen that the saddle point conditions

$$E = -\frac{\partial}{\partial \beta'} ln \mathcal{Z} \tag{9}$$

and

$$N_{p,n} = \frac{\partial}{\partial \alpha_{n,n}} ln \mathcal{Z} \tag{10}$$

are satisfied. The quantity \mathcal{D} in eq. (7) is a determinant of 3×3 matrix defined by the elements

$$d_{ij} = \frac{\partial^2}{\partial x_i \partial x_j} ln \mathcal{Z} \tag{11}$$

where, $x \equiv (\beta', -\alpha_p, -\alpha_n)$ and the second derivatives are evaluated at saddle points. For the sake of comparison with the experiment we present below the results for $\rho(E)$, instead of W(E), which can be obtained as[10],

$$\rho(E) = \frac{W(E)}{\sqrt{2\pi\sigma^2}} \tag{12}$$

where, $\sigma^2 = I^{rig}/\hbar^2$ is the spin cut-off factor with I^{rig} being the rigid - body value of the moment of inertia.

The model space used to perform the numerical calculations is given in Table 1. For the range of temperature $T \leq 2.0~MeV$ this basis space should be adequate. The choice of the values of the spherical single particle energies is a rather difficult task. Due to the quantal nature of the nucleus there is no smooth A-dependence for a large range of A. From our experience in the pf-shell and rare earth region we have finally chosen these numbers with the help of Fig. 1 (suitable for $A \approx 100$) in Ref. [11] and Fig. 1 (suitable for $A \approx 100$) in Ref. [12] which are actually obtained as

solutions of Woods-Saxon potential. The neutron core with N=40 ensures sufficient number of active valance neutrons. The value of the core polarization factor, f_c , is taken to be 1.5. With this the value of the quadrupole deformation parameter, β , in the ground state of ^{104}Pd comes out to be about 0.1 which is quite reasonable [13]. ^{114}Sn is spherical in the ground state. The pairing correlations are also expected to be small for these nuclei.

For the sake of compactness most of our results and discussions will be presented for ^{104}Pd only. For ^{114}Sn results on level densities will be presented towards the end, before conclusions. In Fig. 1 we display the SPA as well as SPA+RPA results for the variation of energy as a function of temperature for ^{104}Pd . To obtain E(T) within the SPA+RPA we first of all check the convergence of the RPA correction factor $\mathcal{C}_{\mathcal{RPA}}$ by choosing various values of N_m in eq. (4). We find that $N_m = 40$ is sufficient but we have used $N_m = 80$ in the present calculation so that at very low temperatures it should be sufficiently accurate. We see that, as in Refs. [9, 14], the RPA or quantal fluctuation corrections lower the value of E(T)at lower temperatures. As temperature increases, quantal fluctuation decreases or $\mathcal{C}_{\mathcal{RPA}} \to \infty$ yielding the value of E(T) close to the one obtained within SPA. However, it shows that the RPA corrections are important up to about T=2MeV. We then next show in Fig. 2 the variation of the level density as a function of E^* . The values of E(0) needed to calculate E^* are obtained in the case of SPA as well as SPA+RPA by extrapolating the corresponding curves of Fig. 1 to T=0. These values come out to be equal to -310.603 and -315.357 MeV in the case of SPA and SPA+RPA, respectively. We see that SPA+RPA results for the level density are in good agreement with the ones extracted recently [7] through the measurements of proton yields in the reaction ${}^{93}Nb({}^{12}C,p){}^{104}Pd$. On the other hand, SPA level densities are higher compared to the measured values. For instance, the ratio $\rho_{SPA}/\rho_{exp}\approx 10^2$ at $E^*=10~MeV$ which reduces to about 10 at $E^* = 24 \; MeV$. Whereas, $\rho_{SPA+RPA}/\rho_{exp}$ varies from 1.0 - 1.2 over the entire

range of E^* for which experimental data are available. It should be mentioned that we have not put the error bars on the experimental data. The experimental data have errors of the order of 20 - 30% at the lower end and of a few percent at the other end.

Next, we now discuss about the parameterization of the SPA+RPA level densities in order to extract a value of the level density parameter, a. We have shown in our earlier work[15] that SPA level density can be reproduced by Bethe's formula provided an appropriate value of the parameter 'a' is used. Normally there are two relations which are used to compute the value of a, namely,

$$E^* = a_e T^2 \tag{13}$$

and

$$S = 2a_s T \tag{14}$$

where, the suffices e and s are used to distinguish the value of a' determined using E^* or S, respectively. Treating a_e and a_s equal, usually a third relation $a = S^2/4E^*$ is also derived. However, in reality there is no rigorous reason to do so. Usually all the three relations yield different values of a when computed numerically. Hence, it becomes a natural question to ask as to which a' is appropriate for the use in Bethe's formula for the level densities [10]:

$$\rho(E) = \frac{\sqrt{\pi}}{12} \frac{e^{2\sqrt{aE^*}}}{a^{1/4} (E^*)^{5/4}} \frac{1}{\sqrt{2\pi\sigma^2}}.$$
 (15)

It is important to realise from eqs. (7 - 9) that the constant part of the prefactor [16] in eq. (2) which normalizes the 'measure' does not contribute to the calculation of E^* but certainly contributes to the value of S. In any mean field approach the effect of this prefactor would be missing. Now using eqs. (13) and (14) we can write

$$S = 2\sqrt{\frac{a_s^2 E^*}{a_e}} = 2\sqrt{aE^*}$$
 (16)

where,

$$a = a_s^2 / a_e = S^2 / 4E^* (17)$$

We find that the values of a required in eq. (15) to get $\rho_{SPA+RPA}$ is quite close to the one given by eq. (17). For instance, at T=0.5, 1.0, 1.5 and 2.0 MeV we get $a(a_{fit})=10.46(11.04), 12.92(13.12), 12.42(12.49), 11.89(11.94), respectively. In Fig. 3 we have displayed the variation of the inverse level density parameter <math>(K=A/a)$ as a function of the excitation energy per particle, $\epsilon=E^*/A$ [17] which correspond roughly to T=0 - 2.0 MeV. The values of K_e , K_s and K_{es} are obtained using 'a' calculated from eqs. (13), (14) and (17), respectively. We see that in comparison to K_e and K_s the values of K_{es} are increasing very slowly with ϵ or temperature for $T \geq 1.0 \ MeV$. Also, we would like to point out that the values of K_{es} are quite close to the experimental values [7] available for $E^*=16-22 \ MeV$. Behaviour of K in the very low temperature region $(T \leq 0.5 MeV)$ is reflecting the well known effects of shell structures.

Finally in Fig. 4 we have displayed the variation of the level density as a function of E^* for ^{114}Sn . The theoretical curves are drawn after dividing the actual numbers by a factor 20.827 such that the upper most point (with minimum uncertainty) of the experimental data matches with the one calculated in the SPA+RPA approach. The variation is rather very well reproduced by the solid curve keeping in mind the fact that the experimental values have also large inherent uncertainties [7]. The SPA curve is roughly parallel to the SPA+RPA one (the ratio $\rho_{SPA}/\rho_{SPA+RPA} \approx 4.5$ at $E^* = 5.0~MeV$ and 2.6 at $E^* = 30~MeV$) emplying that here the variation is approximately reproduced.

In conclusion, we have studied the excitation energy dependence of level densities for ^{104}Pd and ^{114}Sn including thermal as well as quantal fluctuations of the nuclear quadrupole shape parameters. We find that inclusion of quantal fluctuations is essential to reproduce the experimental data even upto the excitation energy of about 25 MeV (or $T \approx 1.5 \ MeV$). We have also shown that the value of

the level density parameter 'a' to be used in the Bethe's formula (eq. (15)) should be computed from eq. (17) only. Also, this value of a can not be used to relate temperature to get S or E^* , particularly in the SPA or SPA+RPA approach. Actually the calculation of a from a_s^2/a_e is essentially equivalent to fitting the value of the level densities to the Bethe's formula.

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Table 1: Spherical single-particle energies (in units of $\hbar\omega_0$) with Z=28 and N=40 as a core for proton and neutron, respectively.

| Protons | | Neutrons | |
|-------------|-------------------|-------------|-------------------|
| Spherical | Energy | Spherical | Energy |
| orbits | $(\hbar\omega_0)$ | orbits | $(\hbar\omega_0)$ |
| $1p_{3/2}$ | -1.376 | $0g_{9/2}$ | -0.975 |
| $0f_{5/2}$ | -1.374 | $1d_{5/2}$ | -0.484 |
| $1p_{1/2}$ | -1.171 | $0g_{7/2}$ | -0.30 |
| $0g_{9/2}$ | -0.975 | $2s_{1/2}$ | -0.216 |
| $1d_{5/2}$ | -0.484 | $1d_{3/2}$ | -0.122 |
| $0g_{7/2}$ | -0.30 | $0h_{11/2}$ | -0.122 |
| $2s_{1/2}$ | -0.216 | $0h_{9/2}$ | 0.358 |
| $1d_{3/2}$ | -0.122 | $1f_{7/2}$ | 0.405 |
| $0h_{11/2}$ | -0.122 | | |

Figure Captions

Figure 1: Variation of energy as a function of temperature.

Figure 2: Variation of the level density as a function of excitation energy. Solid circles represent the experimental values taken from Ref. [7].

Figure 3: Variation of the inverse level density parameter (K = A/a) as a function of $\epsilon = E^*/A$. The curves labelled K_e , K_s and K_{es} are obtained with the values of 'a' calculated using eqs. (13), (14) and (17), respectively.

Figure 4: Excitation energy dependence of level density for ^{114}Sn . Dashed and Solid curves represent the values of SPA and SPA+RPA level density, respectively reduced by a factor of 20.827 (see the text for details).

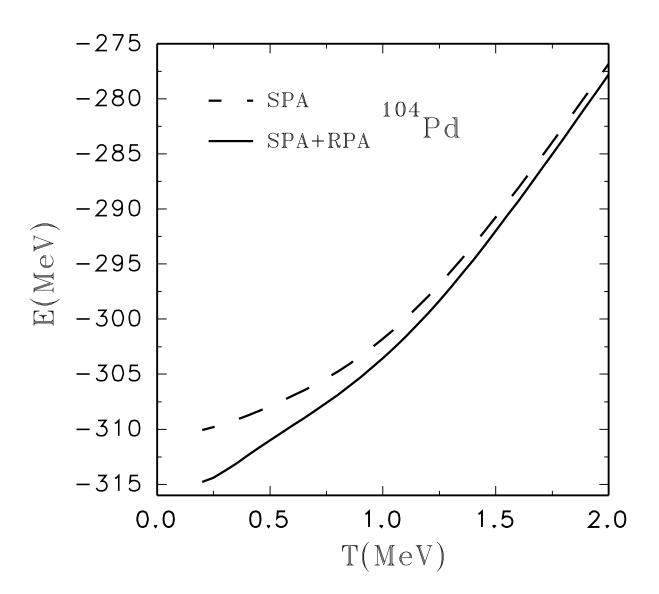


Fig. 1

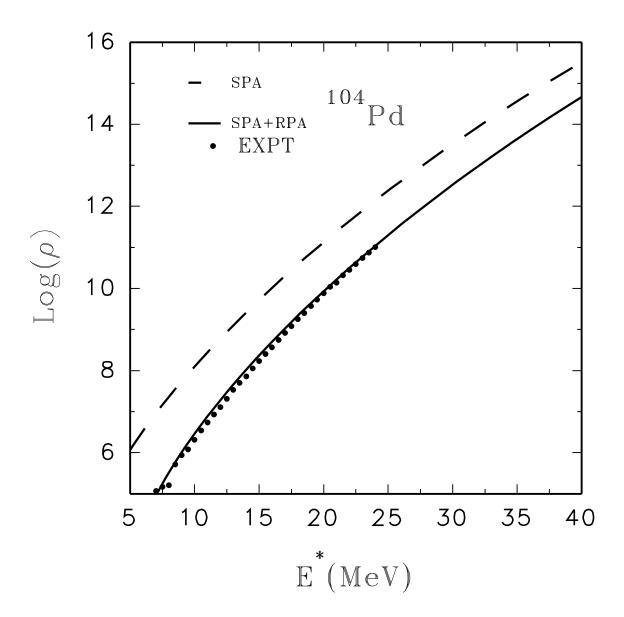


Fig. 2

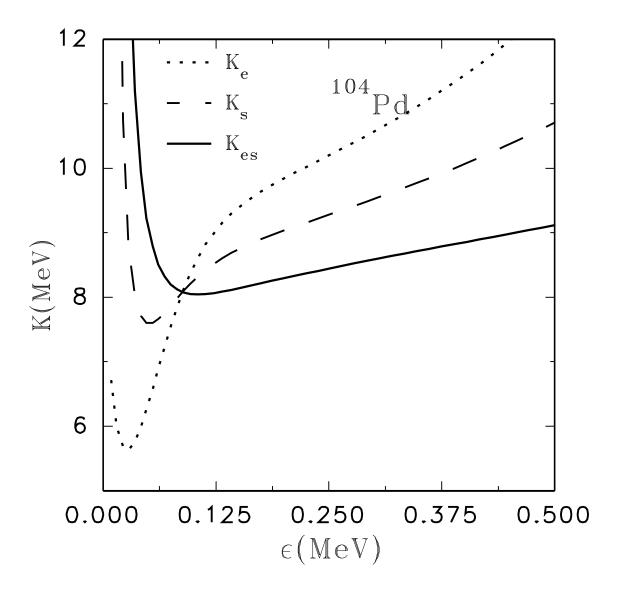


Fig. 3

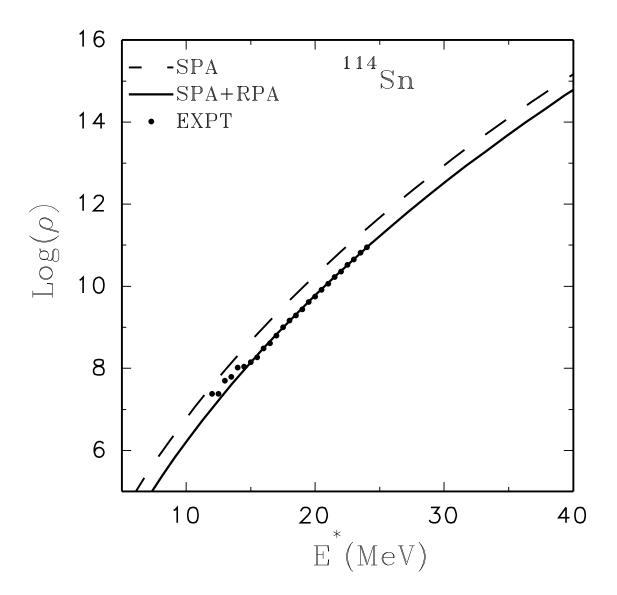


Fig. 4